

# On Effective Hamiltonians for Adiabatic Perturbations of Magnetic Schrödinger Operators

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**Abstract.** *We construct almost invariant subspaces and the corresponding effective Hamiltonian for magnetic Bloch bands. We also discuss the question of the dynamics related to the effective Hamiltonian. We assume that the magnetic and electric potentials are slowly varying perturbations of the potential of a constant magnetic field and a periodic lattice potential, respectively.*

## 1. Introduction

In [5] we constructed wave packets for adiabatic perturbations of Schrödinger operators in periodic media. The recent work of Panati-Spohn-Teufel, [19], led us to consider the relation of those constructions to effective Hamiltonians. In §3 of this article we give a simple derivation of effective Hamiltonians for these problems.

The main simplification in our method is the omission of the Floquet-Bloch transformation. This transformation has many nice properties. In particular, it is unitary, and this makes it useful in studying spectral properties of operators. In the work of Helffer-Sjöstrand [9] and Gérard-Martinez-Sjöstrand [7] this transformation was used quite effectively in the computation of spectra, both of perturbed and effective Hamiltonians. However, if one is simply interested in effective Hamiltonians, the Floquet-Bloch transformation requires that one transform the Hamiltonian by a Fourier integral unitary operator only to transform it back at the end of the calculation. In this article we need to assume that eigenspaces of the unperturbed Hamiltonian depend smoothly on quasi-momentum, and form trivial bundles over a fundamental domain for the dual lattice.

There is also the interesting question of how one interprets the lower order terms in the effective Hamiltonian. If one considers the propagation of observables in the Heisenberg picture, it is natural to think of these terms as lower order corrections to the dynamics. This point of view is adopted in [19], and it is implicit in [3] and [4]. However, the highest order contributions of these terms to the wave packets are in a precession of the phase. Thus in [5] we did not include them in the dynamics, and did not see how to reconcile our results with those of [3] and [4]. It now appears that the two points of view complement each other instead of conflicting.

## 2. Preliminaries

The Hamiltonian for an electron in a crystal lattice  $\Gamma$  in  $\mathbb{R}^3$  in the presence of a constant magnetic field  $\omega = (\omega_1, \omega_2, \omega_3)$  is given by

$$H_0 = \frac{1}{2m} \left( -i\hbar \frac{\partial}{\partial x} + e \frac{\omega \times x}{2} \right)^2 + V(x), \quad (1)$$

where  $V$  is a smooth, real-valued potential, periodic with respect to  $\Gamma$ . Here  $m$  and  $e$  are the mass and charge of the electron. To simplify notation we will use units in which  $\hbar = 2m = e = 1$ .

We will assume that  $\Gamma$  is generated by the basis  $\{e_1, e_2, e_3\}$  for  $\mathbb{R}^3$ ,

$$\Gamma = \{ \sum_{j=1}^3 n_j e_j \mid n_j \in \mathbb{Z} \} \subset \mathbb{R}^3 \quad (2)$$

and let  $E$  be the fundamental domain  $\{\sum_{j=1}^3 t_j e_j, t_j \in [0, 1)\}$ . We will use the dual lattice  $\Gamma^* = e_1^* \mathbb{Z} + e_2^* \mathbb{Z} + e_3^* \mathbb{Z}$ , where  $e_j^* \cdot e_k = 2\pi \delta_{jk}$ , with the fundamental domain  $E^* = \{\sum_{j=1}^3 t_j e_j^*, t_j \in [0, 1)\}$ .

To realize  $H_0$  as a self-adjoint operator in  $L^2(\mathbb{R}^3)$  we define it first on the Schwartz functions  $\mathcal{S}(\mathbb{R}^3)$ , and then take the Friedrichs extension. The resulting operator commutes with the magnetic translations introduced by Zak [24],

$$T_\gamma f(x) = e^{i\langle \omega \times x, \gamma \rangle / 2} f(x - \gamma) \quad (3)$$

for  $\gamma \in \Gamma$ . We assume that

$$\langle \omega, \Gamma \times \Gamma \rangle \subset 4\pi\mathbb{Z}.$$

With this assumption  $G = \{T_\gamma, \gamma \in \Gamma\}$  is an abelian group, and we can reduce  $H_0$  by the eigenspaces of  $G$ , i.e. setting

$$\mathcal{D}_k = \{u \in H_{loc}^2(\mathbb{R}^3), T_\gamma u = e^{-ik \cdot \gamma} u, \gamma \in \Gamma\}, \quad (4)$$

considered as a subspace of  $L^2(E)$ ,  $H_0$  restricted to  $\mathcal{D}_k$  is self-adjoint with compact resolvent. We denote its spectrum by

$$E_1(k) \leq E_2(k) \leq \dots$$

Then by standard results the spectrum of  $H_0$  as an operator in  $L^2(\mathbb{R}^3)$  is equal to

$$\cup_{k \in E^*} \cup_{m=1}^\infty E_m(k).$$

Note that, since  $\mathcal{D}_{k+\gamma^*} = \mathcal{D}_k$  for  $\gamma^* \in \Gamma^*$ ,  $E_m(k + \gamma^*) = E_m(k)$ .

Standard perturbation theory shows that the function  $E_m(k)$  is continuous for  $k \in \mathbb{R}^3$  and real analytic in a neighborhood of any  $k$  such that

$$E_{m-1}(k) < E_m(k) < E_{m+1}(k) \quad (5)$$

The closed interval  $\Lambda_m = \cup_{k \in E^*} E_m(k)$  is known as the “m-th magnetic Bloch band” in the spectrum of  $H_0$ .

In what follows it will be convenient to replace  $H_0$  acting on  $\mathcal{D}_k$  by

$$H_0(k) = e^{-ik \cdot x} H_0 e^{ik \cdot x} = \left( -i \frac{\partial}{\partial x} + \frac{\omega \times x}{2} + k \right)^2 + V(x)$$

with the domain

$$\mathcal{D} = \{u \in H_{loc}^2(\mathbb{R}^3), T_\gamma u = u, \gamma \in \Gamma\}.$$

for all  $k$ . As with  $\mathcal{D}_k$ , we consider  $\mathcal{D}$  as a subspace of  $L^2(E)$ .

**Assumption A.** For a given  $m$  we will assume that  $E_m$  satisfies (5) for all  $k$ .

Under this assumption we can choose the eigenfunction  $\Psi(x, k)$  associated to  $E_m(k)$  to be a real-analytic function of  $k$  with values in  $\mathcal{D}$ , such that

$$H_0(k) \Psi(k) = E_m(k) \Psi(k) \text{ for all } k \quad \int |\Psi(x, k)|^2 dx = 1.$$

**Assumption B.** We assume that

$$\Psi(x, k + \gamma^*) = e^{i\gamma^* \cdot x} \Psi(x, k), \gamma^* \in \Gamma^*.$$

This assumption makes the complex line bundle of the eigenspaces a trivial bundle over the torus,  $\mathbb{R}^3/\Gamma^*$ . In general one has

$$\Psi(x, k + \gamma^*) = e^{i(\gamma^* \cdot x + \theta(k, \gamma^*))} \Psi(x, k), \gamma^* \in \Gamma^*,$$

where  $\theta(k, \gamma^*)$  is real-valued, and determines the structure of the eigenspace bundle. Since

$$\theta(k, m_1 e_1^* + m_2 e_2^* + m_3 e_3^*) = m_1 \theta(k, e_1^*) + m_2 \theta(k, e_2^*) + m_3 \theta(k, e_3^*) \bmod 2\pi,$$

when  $\theta(k, \gamma^*)$  is nonzero, the derivatives of  $\Psi$  with  $k$  will be unbounded and  $\Psi$  will not belong to the class of symbols  $\mathcal{B}$  which we introduce below. Thus we need Assumption B.

**Remark 1.** *The general method of constructing effective Hamiltonians which we give here will apply under the weaker hypothesis: for a given  $m$  there exist  $p$  and  $q$  such that*

$$E_{m-p-1}(k) < E_{m-p}(k) \text{ and } E_{m+q}(k) < E_{m+q+1}(k) \text{ for all } k.$$

*However, in this case the effective Hamiltonian will be a matrix operator acting on functions with values in  $\mathbb{C}^{p+q+1}$ , as in [6], [7], [9] and [19].*

### 3. Main Result

The adiabatically perturbed Hamiltonian is

$$H_\epsilon = \left( -i \frac{\partial}{\partial x} + \frac{\omega \times x}{2} + A(\epsilon x) \right)^2 + V(x) + W(\epsilon x),$$

where  $W$  and  $A = (A_1, A_2, A_3)$  are smooth, and bounded together with all of their derivatives. As before, we define  $H_\epsilon$  first on  $\mathcal{S}(\mathbb{R}^3)$ , and then take the Friedrichs extension to get a self-adjoint operator in  $L^2(\mathbb{R}^3)$ .

The essential step in applying multi-scale techniques is simply to consider  $y = \epsilon x$  as a new independent variable in  $H_\epsilon$ . Let

$$\tilde{H}_\epsilon = \left( -i \frac{\partial}{\partial x} - i\epsilon \frac{\partial}{\partial y} + \frac{\omega \times x}{2} + A(y) \right)^2 + V(x) + W(y).$$

Then, for  $u(x, y)$  we can define  $w(x) = u(x, \epsilon x)$  and conclude that

$$[\tilde{H}_\epsilon u](x, \epsilon x) = [H_\epsilon w](x). \quad (6)$$

The identity (6) enables us to solve the Schrödinger equation for  $H_\epsilon$  uniformly in  $\epsilon$  by solving the Schrödinger equation for  $\tilde{H}_\epsilon$  uniformly in  $(y, \epsilon)$ . The latter might sound more difficult, but it turns out not to be.

Let  $\mathcal{B}$  denote the subspace of  $C^\infty(\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3)$  consisting of functions of the form

$$P(x, y, k, \epsilon) = P_0(x, y, k) + \epsilon P_1(x, y, k) + \cdots + \epsilon^N P_N(x, y, k)$$

such that  $P(x + \gamma, y, k, \epsilon) = e^{i\langle \omega \times x, \gamma \rangle / 2} P(x, y, k, \epsilon)$  and

$$\sup_{y, k} \|\partial_y^\alpha \partial_k^\beta P_j(\cdot, y, k)\|_{L^2(E)} < \infty, \text{ for all } \alpha, \beta \in \mathbb{N}^3.$$

To  $P \in \mathcal{B}$  we associate the  $\epsilon$ -pseudo-differential operator

$$P(x, y, \epsilon D_y, \epsilon) f(x, y, \epsilon) = (2\pi\epsilon)^{-3} \int e^{ik \cdot (y-z)/\epsilon} P(x, y, k, \epsilon) f(z) dz dk, f \in \mathcal{S}(\mathbb{R}^3).$$

Note that here we are using the standard quantization – as opposed to the Weyl quantization. Our main result is the following:

**Theorem.** *For every  $N \in \mathbb{N}$  there exist  $P_N = F_0 + \epsilon F_1 + \cdots + \epsilon^N F_N \in \mathcal{B}$  and  $H_{eff}^N = h_0 + \epsilon h_1 + \cdots + \epsilon^N h_N \in \mathcal{B}$  (independent on  $x$ ) such that*

$$\tilde{H}_\epsilon(P_N(x, y, \epsilon D_y, \epsilon)u) - P_N(x, y, \epsilon D_y, \epsilon)H_{eff}^N(y, \epsilon D_y)u = \mathcal{O}(\epsilon^{N+1}) \quad (7)$$

for  $u \in \mathcal{S}(\mathbb{R}^3)$ . Moreover, considered as an operator from  $L^2(\mathbb{R}^3)$  into  $L^2(E \times \mathbb{R}^3)$ ,  $P_N$  is approximately isometric, i.e.  $P_N^* P_N = I + \mathcal{O}(\epsilon^{N+1})$ .

We interpret  $H_{eff}^N$  as the effective Hamiltonian up to order  $\epsilon^N$ . The leading term in its symbol is  $h_0(y, k) = E_m(k + A(y)) + W(y)$ . This is the well-known “Peierls substitution”, [20]. The symbol of  $h_1$  is also quite interesting, and we discuss it in §4.

**Proof.** As in §2 it will be convenient to work with

$$\tilde{H}_\epsilon(k) = e^{-ik \cdot x} \tilde{H}_\epsilon e^{ik \cdot x} = \left( -i \frac{\partial}{\partial x} - i\epsilon \frac{\partial}{\partial y} + \frac{\omega \times x}{2} + A(y) + k \right)^2 + V(x) + W(y),$$

acting on functions in  $\mathcal{B}$ , in place of  $\tilde{H}_\epsilon$ . Note that

$$\tilde{H}_\epsilon(P_N(x, y, \epsilon D_y, \epsilon)u) = (2\pi\epsilon)^{-3} \int e^{ik \cdot (y-z)/\epsilon} \tilde{H}_\epsilon(k) P_N(x, y, k, \epsilon) u(z) dz dk.$$

The Hamiltonian  $\tilde{H}_\epsilon(k)$  can be written as  $\tilde{H}_\epsilon(k) = \tilde{H}_0(k) + \epsilon \tilde{H}_1(k) + \epsilon^2 \tilde{H}_2(k)$ , where

$$\tilde{H}_0(k) = (-i\partial_x + \frac{\omega \times x}{2} + k + A(y))^2 + V(x) + W(y) = H_0(k + A(y)) + W(y)$$

$$\tilde{H}_1(k) = -2i(-i\partial_x + \frac{\omega \times x}{2} + k + A(y)) \cdot \partial_y - i\partial_y \cdot A(y), \quad (8)$$

and  $\tilde{H}_2(k) = -\Delta_y$ .

We will simply construct the symbols of the pairs  $(h_0, F_0)$ ,  $(h_1, F_1)$ ,  $\dots$ , successively so that (7) holds to order  $\mathcal{O}(\epsilon^{N+1})$  in the  $\epsilon$ -pseudo-differential calculus. To

cancel the order zero terms in (7) we set  $h_0(y, k) = E_m(k + A(y)) + W(y)$  and  $F_0(x, y, k) = \Psi(x, k + A(y))$ . Then, since the symbol of  $F_0(x, y, \epsilon D_y)h_0(y, \epsilon D_y)$  is

$$F_0(x, y, k)h_0(y, k) + \frac{\epsilon}{i} \frac{\partial F_0}{\partial k}(x, y, k) \cdot \frac{\partial h_0}{\partial y}(y, k) + \mathcal{O}(\epsilon^2),$$

we must have

$$(\tilde{H}_0(k) - h_0)F_1 - \frac{1}{i} \frac{\partial F_0}{\partial k} \cdot \frac{\partial h_0}{\partial y} + (\tilde{H}_1(k) - h_1)F_0 = 0. \quad (9)$$

By the Fredholm Alternative in  $L^2(E)$ , we can solve (9) for  $F_1$  if and only if

$$\langle F_0(\cdot, y, k), -\frac{1}{i} \frac{\partial F_0}{\partial k}(\cdot, y, k) \cdot \frac{\partial h_0}{\partial y} + (\tilde{H}_1(k) - h_1(y, k))F_0(\cdot, y, k) \rangle = 0,$$

where  $\langle \cdot, \cdot \rangle$  denotes the inner product in  $L^2(E)$ . Hence, we choose

$$h_1(y, k) = \langle F_0(\cdot, y, k), \frac{-1}{i} \frac{\partial F_0}{\partial k}(\cdot, y, k) \cdot \frac{\partial h_0}{\partial y}(y, k) + \tilde{H}_1(k)F_0(\cdot, y, k) \rangle \text{ and} \quad (10)$$

$$F_1(x, y, k) = (\tilde{H}_0(k) - h_0(y, k))^{-1} \left( \frac{1}{i} \frac{\partial F_0}{\partial k} \cdot \frac{\partial h_0}{\partial y} + h_1 F_0 - \tilde{H}_1(k)F_0 \right) + a_1(y, k)F_0, \quad (11)$$

where  $(\tilde{H}_0(k) - h_0(y, k))^{-1}$  denotes the inverse which maps the orthogonal complement of  $F_0(\cdot, y, k)$  in  $L^2(E)$  onto itself. We recall that

$$\tilde{H}_0(k) - h_0(y, k) = H_0(k + A(y)) - E_m(k + A(y)).$$

We determine  $a_1(y, k)$  by the requirement that  $P_N^* P_N = I + \mathcal{O}(\epsilon^{N+1})$ . Given  $f, g \in \mathcal{S}(\mathbb{R}^3)$ , this implies

$$\begin{aligned} \int_E dx \int_{\mathbb{R}^3} [(\overline{F_0(x, y, \epsilon D_y) + \epsilon F_1(x, y, \epsilon D_y)}) f] [(F_0(x, y, \epsilon D_y) + \epsilon F_1(x, y, \epsilon D_y)) g] dy = \\ \int_{\mathbb{R}^3} \bar{f} g dy + \mathcal{O}(\epsilon^2). \end{aligned} \quad (12)$$

Since  $\int_E |F_0(x, y, k)|^2 dx = 1$  for all  $(k, y)$ , one can calculate  $\text{Re}\{a_1(y, k)\}$  from (12), and see that it is smooth and bounded, by the pseudo-differential calculus. We choose  $\text{Im}\{a_1(y, k)\} = 0$ .

The calculation of  $(F_j, h_j)$  for  $j > 1$  proceeds in the same manner: we calculate the terms of order  $\epsilon^j$  in the symbol of the left hand side of (7) which come from  $(F_l, h_l)$  for  $l < j$  and choose  $(F_j, h_j)$  so that the left hand side of (7) has the desired form up to terms of order  $\epsilon^{j+1}$ . At each stage we use the Fredholm Alternative in  $L^2(E)$ , and  $F_j$  is only determined modulo a term of the form  $a_j(y, k)F_0(x, y, k)$ . Then we choose the real part of  $a_j(y, k)$  so that  $P_j^* P_j = I + \mathcal{O}(\epsilon^{j+1})$ , and take the imaginary part of  $a_j$  to be zero. Continuing in this way we complete the proof of the Theorem.

**Remark 2** If we set  $\Pi_N = P_N P_N^*$ , then  $\Pi_N$  is approximately a projection:  $\Pi_N^2 = \Pi_N + \mathcal{O}(\epsilon^{N+1})$  and  $\Pi_N = \Pi_N^*$ . The equation (7) implies that

$$P_N^* \tilde{U} - \Pi_N - P_N^* = \mathcal{O}(\epsilon^{N+1})$$

Hence

$$P_N P_N^* \tilde{H}_\epsilon = P_N H_{eff} P_N^* + \mathcal{O}(\epsilon^{N+1}).$$

If we replace  $P_N H_{eff}$  in the equality above by the left hand side of (7), we obtain:

$$P_N P_N^* \tilde{H}_\epsilon = \tilde{H}_\epsilon P_N P_N^* + \mathcal{O}(\epsilon^{N+1}).$$

Thus  $\Pi_N$  is a projection which commutes with  $\tilde{H}_\epsilon$  to order  $\mathcal{O}(\epsilon^{N+1})$  as in [19].

In [19], the construction of the almost invariant subspaces is based on the method of Nenciu-Sordani [17] and Sordani [18] (see also [10], [14], [15]). This method is heavily related to the construction of Moyal projections.

#### 4. Relations with Previous Work

To relate the results here to what has already been done we need to complete the calculation of the effective Hamiltonian up to terms of order  $\epsilon^2$ , i.e. to compute the symbol  $h_1(y, k)$  from (10). The explicit computation of

$$\langle F_0(\cdot, y, k), \tilde{H}_1(k) F_0(\cdot, y, k) \rangle =_{def} E_1(y, k)$$

is contained in the computations in [5] (it is also in [8] with a small error – see Remark 1 in [5]). When one replaces  $k(y, s)$  and  $\Psi(x, y, s)$  in [5, pp. 7601-3] by  $k + A(y)$  and  $\Psi(x, k + A(y))$  respectively,  $E_1(y, k)$  is “ $i\hbar$ ” in the notation of [5, (25)] and we have

$$E_1 = \frac{1}{2i} \frac{\partial}{\partial y} \cdot \frac{\partial E_m(\tilde{k})}{\partial k} - L \cdot B - i \langle \Psi(\cdot, \tilde{k}), \frac{\partial \Psi(\cdot, \tilde{k})}{\partial y} \rangle \cdot \frac{\partial E_m(\tilde{k})}{\partial k},$$

where  $\tilde{k} = k + A(y)$ . Here  $B(y) = \nabla \times A(y)$  and  $L =$

$$L = \text{Im} \left( \langle M(y, k) \frac{\partial \Psi}{\partial k_2}, \frac{\partial \Psi}{\partial k_3} \rangle, \langle M(y, k) \frac{\partial \Psi}{\partial k_3}, \frac{\partial \Psi}{\partial k_1} \rangle, \langle M(y, k) \frac{\partial \Psi}{\partial k_1}, \frac{\partial \Psi}{\partial k_2} \rangle \right).$$

with  $M(y, k) = \tilde{H}_0(k) - h_0(y, k)$ . The vector  $L$  is an angular momentum and  $L \cdot B$  contributes the “Rammal-Wilkinson” term to the energy, cf. [1]. Adding the additional term from (10) to  $E_1$  to obtain  $h_1$ , we obtain

$$h_1(y, k) = \frac{1}{2i} \frac{\partial}{\partial y} \cdot \frac{\partial E_m(k + A(y))}{\partial k} - L \cdot B - i \langle \Psi(\cdot, k + A(y)), \dot{\Psi}(\cdot, k + A(y)) \rangle, \quad (13)$$

where

$$\dot{\Psi}(x, k + A(y)) = \frac{\partial \Psi(x, k + A(y))}{\partial y} \cdot \dot{y} + \frac{\partial \Psi(x, k + A(y))}{\partial k} \cdot \dot{k}$$

and  $\dot{y}$  and  $\dot{k}$  are defined by the Hamiltonian system

$$\dot{y} = \frac{\partial(E_m(k + A(y)) + W(y))}{\partial k} \quad \dot{k} = -\frac{\partial(E_m(k + A(y)) + W(y))}{\partial y}.$$

Thus one recognizes  $i \langle \Psi(\cdot, k + A(y)), \dot{\Psi}(\cdot, k + A(y)) \rangle$  as the term generating the Berry phase precession, cf. [13], [22]. Comparing (13) with [19, (22)] (in the case  $l = 1$ ), one sees that they agree completely when one takes into account the difference in

the choice of sign in the magnetic potential,  $A(y)$ , and the use of Weyl quantization in [19]. The sign of the Berry phase term in (13) may appear inconsistent with [5, (29)], but it is not. In [5]  $(\dot{y}, \dot{k})$  was the vector field from the Hamiltonian  $-E_m(k + A(y))$ .

In [5] and [8] instead of introducing effective Hamiltonians we constructed wave packets. These packets are nonetheless related to effective Hamiltonians in that one can compute what the effective Hamiltonian must be – assuming that there is one – from the packets. To see this one can proceed as follows. The packets have the form (here  $s = \epsilon t$  and  $W(y) = 0$ )

$$u(x, y, s, \epsilon) = e^{i\phi(y, s)/\epsilon} [f(y, s)\Psi(x, \frac{\partial\phi}{\partial y} + A(y)) + \mathcal{O}(\epsilon)],$$

where  $\phi$  and  $f$  are solutions of

$$\frac{\partial\phi}{\partial s} = E_m(\frac{\partial\phi}{\partial y} + A(y)) \text{ and } \frac{\partial f}{\partial s} = \frac{\partial E_m}{\partial k}(\frac{\partial\phi}{\partial y} + A(y)) \cdot \frac{\partial f}{\partial y} + (D - iL \cdot B + \langle \Psi, \dot{\Psi} \rangle) f. \quad (14)$$

Here all functions of  $(k, y)$  are evaluated at  $k = \tilde{k}(y, s) = \partial_y \phi$ , and  $D = (1/2)\partial_y \cdot (\partial_k E_m(\partial_y \phi + A(y)))$ . Assuming that the evolution of  $f$  is governed by an effective Hamiltonian  $H_{eff} = h_0(y, \epsilon D_y) + \epsilon h_1(y, \epsilon D_y) + \mathcal{O}(\epsilon^2)$ , we must have (on bounded intervals in  $s$ )

$$[e^{isH_{eff}/\epsilon} e^{i\phi(\cdot, 0)/\epsilon} f(\cdot, 0)](y, s) = e^{i\phi(y, s)/\epsilon} f(y, s) + \mathcal{O}(\epsilon^2). \quad (15)$$

Differentiating (15) with respect to  $s$ , one concludes

$$\frac{i}{\epsilon} H_{eff}(e^{i\phi(y, s)/\epsilon} f(y, s)) = (\frac{i}{\epsilon} \frac{\partial\phi}{\partial s} f + \frac{\partial f}{\partial s}) e^{i\phi(y, s)/\epsilon} + \mathcal{O}(\epsilon). \quad (16)$$

Using the symbol expansion from the pseudo-differential calculus

$$e^{-i\phi/\epsilon} H_{eff}(e^{i\phi/\epsilon} f) = h_0(y, \tilde{k}) + \epsilon [\frac{1}{i} \frac{\partial h_0}{\partial k}(y, \tilde{k}) \cdot \frac{\partial f}{\partial y}(y) + \frac{1}{2i} \sum_{j,l} \frac{\partial^2 h_0}{\partial k_j \partial k_l}(y, \tilde{k}) \frac{\partial^2 \phi}{\partial y_j \partial y_l}(y) + h_1(y, \tilde{k})] f(y) + \mathcal{O}(\epsilon^2). \quad (17)$$

Substituting (17) into (16) and comparing the result with (14), one recovers the formulas given earlier for  $h_0(y, k)$  and  $h_1(y, k)$ .

In [8] we were unable to reconcile our results with those of Chang and Niu, see [3], [4] and also [23]). We thought that this might have resulted from different choices of scales. This is partially true, since Chang and Niu do not distinguish the scale  $y = \epsilon x$ , but, as Panati, Spohn and Teufel point out in [19], the differences largely disappear when one considers the Heisenberg formulation of quantum dynamics. Letting  $a(y, \epsilon D_y)$  be an observable, the propagation of  $a$  in the Heisenberg picture is given by

$$a(s) = e^{-isH_{eff}/\epsilon} a e^{isH_{eff}/\epsilon} \text{ or } \epsilon \frac{da}{ds} = i[a, H_{eff}].$$

If one considers this propagation at the symbol level, then the symbol of  $a$  is propagating along the trajectories of the Hamiltonian system

$$\dot{y} = \frac{\partial H_{eff}}{\partial k}, \quad \dot{k} = -\frac{\partial H_{eff}}{\partial y}.$$

Hence one can consider the contribution of  $h_1$  as an order  $\epsilon$  correction to the classical Peierls dynamics arising from  $h_0$ . This is the point of view taken in [19]. However, it is worth noting that the wave packets are propagating along the trajectories from  $h_0$  with a precession in their phases arising from (the imaginary part of)  $h_1$ .

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